Quaderni del Dipartimento di Matematica, Università di Modena e Reggio Emilia, n. 61, March 2005.

Additive Operator Splitting Methods for Solving Systems of Nonlinear Finite Difference Equations*

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Abstract

There exists a considerably body of literature on the development, analysis and implementation of multiplicative and additive operator splitting methods for solving large and sparse systems of finite difference equations arising from the discretization of partial differential equations.
In this note, we will review the Newton–Arithmetic Mean and the Modified Newton–Arithmetic Mean methods for solving nonlinear and weakly nonlinear systems of difference equations arising from the discretization of diffusion–convection problems.

Key Words: Newton–iterative methods, Arithmetic Mean method, finite differences.

AMS Classification: 65H10, 65M20.

C.R. Categories: G.1.8, G.1.5.

1 Statement of the problem

Many problems related to the study of diffusion convection processes in a medium occupying a region R are described by the nonlinear differential equation of parabolic type

$$\frac{\partial\varphi}{\partial t} = \operatorname{div}(\sigma(\varphi)\operatorname{grad}\varphi) + v\cdot\operatorname{grad}\varphi - f(x,t,\varphi(x,t)) \qquad x\in R; t>0 \tag{1}$$

subject to an initial condition

$$\varphi(x,0) = h(x) \qquad x\in\bar{R} \tag{2}$$

*This work was communicated at the intenational INdAM Summer School on "Numerical Methods for Local and Global Optimization: Sequential and Parallel Algorithms", Cortona, Italy, July 14–18, 2003.

and a boundary condition of the mixed form

$$\alpha\varphi(x,t) + \beta\frac{\partial\varphi(x,t)}{\partial\nu} = g(x,t) \tag{3}$$

specified at each point of ∂R, the boundary of the domain R; $\partial\varphi/\partial\nu$ is the directional derivative of φ in the direction ν.
The diffusion coefficient $\sigma(\varphi)$ and the term $f(x,t,\varphi(x,t))$ are real–valued sufficiently smooth functions; besides $\sigma(\varphi) > 0$ in R.
For computational purpose, the parabolic equation (1), when the vector velocity v dominates σ, must be treated as being of hyperbolic type. We will consider only the diffusion–dominated case.
The nonlinearity introduced by the φ–dependence of the functions $\sigma(\varphi)$ and $f(x,t,\varphi)$ requires that, in general, the solution to equation (1) be approximated by numerical methods.
The method of finite differences is a popular numerical method for estimating the solution to a problem of the form (1)–(3).
Problems of thermal ignition and combustion, of chemical reaction and of population growth lead to a diffusion–convection equation (1).
Generally, we solve these problems with an *implicit finite difference method.*
By an implicit finite difference method for equation (1) we mean the approximation of the time derivative by a suitable backward difference quotient. The parabolic equation (1) is thus replaced by sequence of elliptic partial differential equations which we shall write as

$$-\mathrm{div}(\sigma(x,t_l,\varphi(x,t_l))\mathrm{grad}\varphi(x,t_l) + \gamma(x,t_l,\varphi(x,t_l))\cdot\varphi(x,t_l) + \psi(x,t_l,\varphi(x,t_l)) = 0 \tag{4}$$

where $\{t_l\}$ denotes an increasing sequence of discrete time values, and, where the source term $\psi(x,t_l,\varphi(x,t_l))$ includes the data and the history of the evolution system.
It is experimentally observed and really proved for linear equations, that the solution of a parabolic equation by a sequence of elliptic equations is not subject to stability restriction on the admissible time–step. This is an essential feature since in many applications the behaviour of a diffusion–convection problem has to be modelled over long time periods with fine spatial resolution.
Now, the discretization of the spatial derivatives at each time value t_l leads to the solution of a sequence of nonlinear algebraic systems of large dimensions.
Thus, at a fixed discrete time value t_l, equation (4) is transformed into a system of n nonlinear equations of the form

$$F(u) \equiv A(u)u + G(u) = 0 \tag{5}$$

where $A(u)$ is an $n \times n$ sparse matrix.
Computing the solution u of (5) is very expensive for n large. This a serious drawback for the implicit finite difference method; the computational complexity of the method is very high.
This occurrence has been known since the early days of numerical solution to parabolic partial differential equations. The work of Peaceman and Rachford

([19]) is a famous example for overcoming this difficulty by *operator splitting methods*.
For example, if we can decompose the jacobian matrix $F'(u)$ of the mapping $F(u)$ in the form

$$F'(u) = H(u) + V(u) \tag{6}$$

for all u in an open neighbourhood Ω_0 of a root u^* of $F(u) = 0$, we can define the following nonlinear *Alternating Direction Implicit* (ADI) iterative method

$$u^{(k+1)} = u^{(k)} - 2\rho(V(u^{(k)}) + \rho I)^{-1}(H(u^{(k)}) + \rho I)^{-1}F(u^{(k)}) \tag{7}$$

for $k = 0, 1, ...$; $\rho > 0$, which, under standard assumptions generates a sequence $\{u^{(k)}\}$ of iterates converging to the root u^*.
Theorem 1. Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a Fréchet differentiable on an open neighbourhood Ω_0 of a point u^* such that $F(u^*) = 0$. Let $H(u)$ and $V(u)$ be two matrices such that splitting (6) holds for all $u \in \Omega_0$.
Suppose that $H(u)$ and $V(u)$ are continuous at u^*, that $H(u^*) + H(u^*)^T$ and $V(u^*)+V(u^*)^T$ are positive semidefinite, and that at least one of them is positive definite.
Then, for any $\rho > 0$, u^* is a point of attraction of the iteration (7), that is, there is an open neighbourhood Ω of u^* such the $\Omega \subset \Omega_0$ and, for any $u^{(0)} \in \Omega$, the iterates $\{u^{(k)}\}$ defined by (7) all lie in Ω and converge to u^*.
This result extends Theorem 10.3.8 in [18, p. 328].

2 The Newton–Iterative Method for Nonlinear Finite Difference Systems

A very important method for the solution of large systems of nonlinear difference equations of the form (5) is the Newton–iterative method.
At each stage k of Newton's method, the Newton equation

$$F'(u^{(k)})\Delta u = -F(u^{(k)}) \tag{8}$$

must be solved. Computation of the exact solution can be expensive when n is large and, for any n, may not be justified when $u^{(k)}$ is relatively far from u^*. Therefore, we compute an approximate solution of (8) by performing some iterations of an *inner* linear iterative solver, such as SOR, for the equation (8).
In [10] we have considered the *Newton–Arithmetic Mean method* which incorporates at each stage k of Newton's method the Arithmetic Mean (AM) method as inner iterative solver for equation (8).
This method is particularly well suited for implementation on a parallel computer when the jacobian matrix $F'(u)$ is a real nonsingular $T(q, r)$ matrix $(1 \leq q \leq m - 1;\ 1 \leq r \leq m - 1)$, as those arising from the discretization of elliptic boundary value problems; the block tridiagonal matrix $A(u)$ in formula

(5) belongs to the class $T(1,1)$.

$$F'(u) = \begin{pmatrix} J_{1,1}(u) & \cdots & J_{1,r+1}(u) & & & & \\ \vdots & \ddots & & & \ddots & & \\ J_{q+1,1}(u) & & \ddots & & & \ddots & \\ & \ddots & & & \ddots & & J_{m-r,m}(u) \\ & & \ddots & & & \ddots & \vdots \\ & & & & J_{m,m-q}(u) & \cdots & J_{m,m}(u) \end{pmatrix}$$

Each square block $J_{i,j}(u)(i,j=1,...,m)$ is a matrix of order $\tilde{m}$; thus $n = m \cdot \tilde{m}$. We consider the following two splittings of the matrix $F'(u)$:

$$F'(u) = M_1(u) - N_1(u) = M_2(u) - N_2(u) \tag{9}$$

where, if m is even

$$M_1(u) = \begin{pmatrix} J_{1,1}(u) & J_{1,2}(u) & & & & & \\ J_{2,1}(u) & J_{2,2}(u) & & & & & \\ & & J_{3,3}(u) & J_{3,4}(u) & & & \\ & & J_{4,3}(u) & J_{4,4}(u) & & & \\ & & & & \vdots & & \\ & & & & & J_{m-1,m-1}(u) & J_{m-1,m}(u) \\ & & & & & J_{m,m-1}(u) & J_{m,m}(u) \end{pmatrix}$$

and, consequently

$$N_1(u) = M_1(u) - F'(u)$$

$$M_2(u) = \begin{pmatrix} J_{1,1}(u) & & & & & & \\ & J_{2,2}(u) & J_{2,3}(u) & & & & \\ & J_{3,2}(u) & J_{3,3}(u) & & & & \\ & & & \vdots & & & \\ & & & & J_{m-2,m-2}(u) & J_{m-2,m-1}(u) & \\ & & & & J_{m-1,m-2}(u) & J_{m-1,m-1}(u) & \\ & & & & & & J_{m,m}(u) \end{pmatrix}$$

and,

$$N_2(u) = M_2(u) - F'(u)$$

If m is odd, we can proceed in a similar way.

The splittings (9) allow to define the following Newton–AM method

$$
\begin{array}{l}
\text{choose the initial guess } u^{(0)} \\
\left|\begin{array}{l}
\text{for } k = 0, 1, \ldots \text{ until convergence do} \\
w_k^{(0)} = u^{(k)} \\
\left|\begin{array}{l}
\text{for } j = 1, \ldots, j_k \text{ do} \\
M_1(u^{(k)})z_1 = N_1(u^{(k)})w_k^{(j-1)} - F(u^{(k)}) \\
M_2(u^{(k)})z_2 = N_2(u^{(k)})w_k^{(j-1)} - F(u^{(k)}) \\
w_k^{(j)} = \frac{1}{2}(z_1 + z_2)
\end{array}\right. \\
u^{(k+1)} = u^{(k)} + w_k^{(j_k)}
\end{array}\right.
\end{array}
\tag{10}
$$

Here $\{j_k\}$ denotes a sequence of positive integers.
The loop over j defines the Arithmetic Mean (AM) method. This method has within its overall mathematical structure certain well defined substructures that can be executed simultaneously. An evaluation of the effective performance of the method on different parallel architectures is reported in papers [21], [11], [12], [13].
The test for termination of the loop over j may be also check of the condition on the residual

$$\|F'(u^{(k)})w_k^{(j)} + F(u^{(k)})\| \leq \eta_k \|F(u^{(k)})\| \tag{11}$$

with $\eta_k \in [0, 1)$ the forcing term.
The convergence of the Newton–AM method has been analyzed for a class of systems whose jacobian matrix satisfies an affine invariant Lipschitz condition. Also a damping technique has been introduced in the method in order to improve the likelihood of convergence from initial approximations that may be outside the attraction ball of the Newton–AM method ([10]).
The peculiar characteristics of the method are highlighted by some computational experiments on representative problems (see [10]).

3 The Modified Newton–Iterative Method for Weakly Nonlinear Finite Difference Systems

In many problems of practical interest the mapping $F(u)$ in (5) has the form

$$F(u) = Au + G(u) \tag{12}$$

where A is a constant nonsingular matrix and $G(u)$ is continuously differentiable mapping with $G'(u)$ invertible for all $u \in \mathbb{R}^n$.

Precisely, the matrix A in (12) is irreducibly diagonally dominant [1] and has positive diagonal entries for all mesh–spacings sufficiently small. Thus, A is an irreducible M–matrix ([22, p. 85], [17, p. 108]).
The vector $G(u)$ can be written as

$$G(u) = Bg(u) + s \tag{13}$$

where B is a constant nonsingular and nonnegative matrix, $s \in \mathbb{R}^n$ is a constant vector and $g(u)$ is a continuously differentiable diagonal mapping, i.e., a non-linear mapping whose i–th component g_i is a function of only the i–th variable u_i for $i = 1, ..., n$.
Typical expressions of $g_i(u_i)$ are the following:

1. Enzyme–substrate reaction model ([15], [16]):

$$g_i(u_i) = \frac{au_i}{1 + bu_i} \qquad a, b > 0$$

($g_i'(u_i) = a/(1 + bu_i)^2$; $g_i(u_i) \geq 0$ and $g_i'(u_i) \geq 0$ for $u_i \geq 0$)

2. Chemical reaction model ([1]):

$$g_i(u_i) = -\tilde{a}(\tilde{c} - u_i)e^{(-\tilde{b}/(1+u_i))} \qquad \tilde{a}, \tilde{b}, \tilde{c} > 0$$

$(g'(u_i) = \tilde{a}(1 + u_i)^{-2}e^{(-\tilde{b}/(1+u_i))}(u_i^2 + (\tilde{b} + 2)u_i + (1 - \tilde{b}\tilde{c})))$

3. Spatially distributed communities model ([5]):

$$g_i(u_i) = \frac{a_1 u_i^2}{b_1 + u_i} \qquad a_1, b_1 > 0$$

or

$$g_i(u_i) = a_2 u_i log(1 + u_i) \qquad a_2 > 0$$

4. Fischer's population growth model ([16]):

$$g_i(u_i) = -a_3 u_i(u_i - \theta)(1 - u_i) \qquad a_3 > 0, \quad 0 < \theta < 1$$

5. Budworm population dynamics model ([16]):

$$g_i(u_i) = -\frac{u_i^2}{1 + u_i} + ru_i(1 - \frac{u_i}{q}) \qquad r, q > 0,$$

6. Radiation model:

$$g_i(u_i) = \lambda e^{(\alpha u_i)} \qquad \lambda, \alpha > 0$$

[1] See [22, p. 23] for the definition of irreducibly diagonally dominant matrix.

7. Molecular interaction model ([20]):

$$g_i(u_i) = u_i^2$$

Moreover, for mesh–spacings sufficiently small, the matrix $F'(u) = A + Bg'(u)$ can be assumed to be an irreducible M–matrix.
A standard assumption for weakly nonlinear partial difference equations of elliptic type as (12)–(13) is the following (see e.g. [18]):
Assumption A. A is a monotone matrix (see [14, p. 360]), B is a nonsingular and nonnegative matrix; $g(u)$ is continuously differentiable diagonal mapping with $0 \leq G'(u) \leq P$ for all $u \in \mathbb{R}^n$ and P positive matrix.
About the existence and the uniqueness of a solution u^* of the system

$$F(u) \equiv Au + Bg(u) + s = 0 \tag{14}$$

we have the following result:
Theorem 2. Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a mapping of the form (12)–(13) on which the Assumption A holds.
If $A^{-1}P$ has spectral radius $\rho(A^{-1}P) < 1$, then the system (14) has a unique solution $u^* \in \mathbb{R}^n$.
At present there exists a lot of interest in two–stage splitting methods for solving the weakly nonlinear system (14), mainly because these methods are greatly suitable for implementation on parallel computers (see e.g. [2], [3], [4], [23]).
These methods are strictly related to the *Modified Newton–AM method* which incorporates at each stage k of the Newton's method the Arithmetic Mean (AM) method as inner iterative solver for the equation (8) and replaces at each stage k the jacobian matrix $F'(u^{(k)})$ in equation (8) with the constant matrix $C = F'(u^{(0)})$. Here, $u^{(0)}$ is the initial approximation to u^*.
The special form (12) of $F(u)$ leads to the following Newton's equation

$$(A + G'(u^{(k)}))u^{(k+1)} = -G(u^{(k)}) + G'(u^{(k)})u^{(k)} \tag{15}$$

The assumption that $F'(u^{(k)}) = C$ for all k modifies equation (15) into

$$Cu^{(k+1)} = -G(u^{(k)}) + Du^{(k)} \tag{16}$$

with

$$G'(u^{(0)}) = F'(u^{(0)}) - A = C - A = D$$

The assumption that $C = F'(u^{(0)})$ may be decomposed into two splittings of type (9)

$$C = M_1 - N_1 = M_2 - N_2 \tag{17}$$

where $M_1 = M_1(u^{(0)})$, $M_2 = M_2(u^{(0)})$, $N_1 = N_1(u^{(0)})$, $N_2 = N_2(u^{(0)})$, leads to the following Modified Newton–AM method

$$
\begin{array}{l}
\text{choose the initial guess } u^{(0)} \\
\left|\begin{array}{l}
\text{for } k = 0, 1, \dots \text{ until convergence do} \\
z_k^{(0)} = u^{(k)} \\
\left|\begin{array}{l}
\text{for } j = 1, \dots, j_k \text{ do} \\
M_1 \tilde{z}_1 = N_1 z_k^{(j-1)} + (Du^{(k)} - G(u^{(k)})) \\
M_2 \tilde{z}_2 = N_2 z_k^{(j-1)} + (Du^{(k)} - G(u^{(k)})) \\
z_k^{(j)} = \frac{1}{2}(\tilde{z}_1 + \tilde{z}_2)
\end{array}\right. \\
u^{(k+1)} = z_k^{(j_k)}
\end{array}\right.
\end{array}
\tag{18}
$$

Here $\{j_k\}$ denotes a sequence of positive integers.
If we set

$$M^{-1} = \frac{1}{2}(M_1^{-1} + M_2^{-1}) \tag{19}$$

$$
\begin{aligned}
H &= \frac{1}{2}(M_1^{-1}N_1 + M_2^{-1}N_2) = \frac{1}{2}(M_1^{-1}(M_1 - C) + M_2^{-1}(M_2 - C)) \\
&= I - M^{-1}C
\end{aligned}
\tag{20}
$$

at each outer iteration k, the Arithmetic Mean method generates for $j = 1, \dots, j_k$ the vectors

$$z_k^{(j)} = H z_k^{(j-1)} + M^{-1}(Du^{(k)} - G(u^{(k)}))$$

Thus,

$$u^{(k+1)} = H^{j_k} u^{(k)} + \left(\sum_{j=0}^{j_k - 1} H^j \right) M^{-1}(Du^{(k)} - G(u^{(k)}) \tag{21}$$

An useful criterion that helps us to decide whether H is convergent is provided by the following theorems ([21]).

Proposition 1. Let C be a strictly or irreducibly diagonally dominant symmetric matrix with positive diagonal entries. Then, the matrices M_1, M_2 and M are nonsingular and the matrix H is convergent.

Proposition 2. Let C be a strictly or irreducibly diagonally dominant matrix with positive diagonal entries and nonpositive off–diagonal entries. Then, the matrices M_1, M_2 and M are nonsingular and the matrix H is convergent.

The above splitting of C is a variant in the block diagonal part of the Alternating Group Explicit (AGE) decomposition introduced by Evans (see i.e. [6], [7]).

The loop over j in (18) defines the Arithmetic Mean (AM) method. This method is ideally suited for implementation on a parallel computer.
An evaluation of the effective performance of the AM method on different parallel architectures is reported in the papers [21], [11], [12], [13].
The stopping criterion used for the Modified Newton–AM method (18) is

$$\|F(u^{(k)})\| \leq \tau_r \|F(u^{(0)})\| + \tau_a$$

with τ_r and τ_a prespecified tolerances.
A convergence theory for method (18) has been developed in [9] when the finite difference equations (12)–(13) satisfy Assumption A.
Theorem 3. Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a mapping of the form (12)–(13) on which the Assumption A holds. Suppose that the matrix AP^{-1} has spectral radius $\rho(AP^{-1}) < 1$ and the matrix $C = F'(u^{(0)})$ with $u^{(0)} \in \mathbb{R}^n$ is a monotone matrix. Let two splittings be defined by $C = M_1 - N_1 = M_2 - N_2$ (M_1 and M_2 nonsingular) with $M_1^{-1} \geq 0$, $M_1^{-1}N_1 \geq 0$ and $M_2^{-1} \geq 0$, $M_2^{-1}N_2 \geq 0$.
Then, for any starting point $u^{(0)} \in \mathbb{R}^n$ and any j_k ($k = 0, 1, \ldots$), the sequence $\{u^{(k)}\}$ generated by the Modified Newton–AM method (18) converges to the solution u^* of $F(u) = 0$.
A result concerning with the monotone convergence of the method (18) is the following theorem.
Theorem 4. Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a mapping of the form (12)–(13) where the jacobian matrix $F'(u) = A + G'(u)$ is a monotone matrix for all $u \in \mathbb{R}^n$, B is a nonsingular and nonnegative matrix and $g(u)$ is a continuously differentiable mapping on $\mathbb{R}^n$.
Assume that a solution u^* of equation (14) exists in $\mathbb{R}^n$ and that, in addition, $G'(u) \geq 0$ for all $u \in \mathbb{R}^n$ and $G'(u)$ satisfies the isotonicity condition $G'(u) \leq G'(v)$ whenever $u \leq v$.
Let C be the matrix $C = F'(u^{(0)})$, where $u^{(0)} \in \mathbb{R}^n$ is a point satisfying the condition $F'(u^{(0)}) \geq 0$, and let two splittings be defined by $C = M_1 - N_1 = M_2 - N_2$ (M_1 and M_2 nonsingular) with $M_1^{-1} \geq 0$, $M_1^{-1}N_1 \geq 0$ and $M_2^{-1} \geq 0$, $M_2^{-1}N_2 \geq 0$.
Then, the sequence $\{u^{(k)}\}$ generated by the Modified Newton–AM method (18), starting from $u^{(0)}$, with the number of iterations j_k fixed at each stage k, satisfies

$$u^* \leq u^{(k+1)} \leq u^{(k)} \qquad k = 0, 1, \ldots$$

A similar result about the monotone convergence of the method (18) has been proved in [8]. In this paper we have considered a parametrized system of weakly nonlinear equations which arises in the computation of the steady spatial distribution of a population of diffusing consumers (predators) in a special resource–consumer (prey–predator) ecological system ([5]).
Positive solutions of the system (14) are of interest to us. A characterization of this positive solution has been obtained.
An application of the method (18) for solving a real practical problem is described in section 4 of [8].

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